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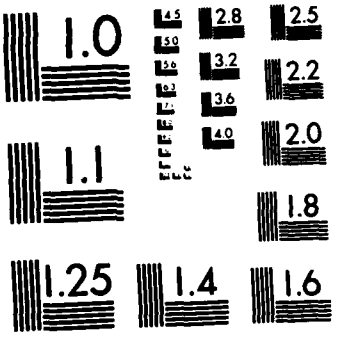

FINAL REPORT

to the

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH

Directorate of Chemical Sciences

Contract # F49620-83-K-0017

on

Collisional Energy Exchange in Polyatomic Molecules

by

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Fourier Transform Infrared Spectrometry (FTIS) has been used to study several kinds of gas-gas and gas-surface collision processes brought about with and in supersonic free jets in vacuo. Following are some key results: (1) Terminal distributions of rotational energy in free jets of CO and CO_2 show a non-Boltzmann distribution that can be characterized by a two-temperature model and explained in terms of competition between rotation-rotation and rotation-translation transfers. (2) Spectra of CO_2 molecules excited by collisions with N_2 molecules indicated similar two-temperature distributions, possibly due

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to secondary collisions between excited CO_2 and N_2. (3) The accommodation of vibrational and rotational energy during collisions between CO, CO_2 and NO molecules and hot platinum surfaces has been determined over a range of surface temperatures. (4) Excess internal energies have been determined in nascent CO and CO_2 molecules formed respectively by catalytic oxidation of C and CO on a platinum surface. An energy balance indicates that about 1/3 of the available reaction energy is absorbed by the surface, the remainder going mostly into vibrational modes of product molecules.

I. Introduction

For the past three years under this grant we have been pursuing a program of research relating to the details of energy exchange processes during collisions between molecules in the gas phase and between molecules and surfaces. This research has been characterized by a combination of methods based on supersonic free jet expansions in vacuo and molecular beam methods with spectroscopy. In particular, we use supersonic free jets expanding into vacuo to bring about the collisions and Fourier Transform Infrared Spectrometry to determine the states of one or both collision partners before and/or after the encounter. In what follows we will set forth briefly what we have been able to accomplish in each of the several topics that we have investigated.

II. Achievements and Results

Reference is made to the Final Technical Report on Contract F49620-80-C-0026 that was submitted three months agon on 21 August 1983. It contained a complete account of our achievements during the period from 1 October 1979 to 21 August 1983. The first three years of that period were under Grant No. F49620-80-C-0026. A one-year grant (No. F49620-83-K-0017) was the instrument for the final year that ended 31 December 1983. This report is the final report on the latter grant. Because the above-mentioned report covered all results up to 21 August 1983, this report covers only the period from 21 August 1983 to 30 December 1983.

During that last four months we continued our time-resolved surface scattering studies of CO oxidation on a platinum surface. We were able to increase the resolution to about 15 microseconds from the 45 microseconds

achieved in the first experiments. There is much information to be extracted from these time-resolved spectra and we are busily engaged in analyzing the data. What clearly emerges thus far in the case of platinum is that the rotational envelope of the nascent CO_2 product molecules is substantially narrower when the surface coverage of oxygen is low. In other words, the rotational "temperature" of the produce molecules is lower when there is less oxygen on the surface. In the case of a palladium surface, on the other hand, there was no difference in rotational "tempeature" as the oxygen coverage of the surface changed. We do not yet understand the implications of these observations. We hope to continue the experiments and to decipher what they are trying to tell us.

There have been no further publications during this four-month period.

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